The NASA Workflow Tool: Project Overview

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What is a Workflow Tool?



A system that provides end-to-end support for setting up and running complex model experiments.

Enable users to concentrate on the scientific results rather than the system environments.



Overview of the NASA Workflow Tool



- Modern GUI tool that provides clear display of options
- Easily configure, run and monitor model experiments
- Detect configuration errors before submitting them
- Automate the complex tasks required to run
- Save experiment configurations for repeatable experiments and sharing experiments between users

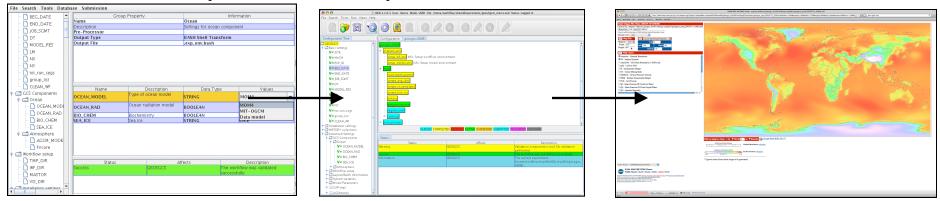
Name	Description	Data Type	Values
OCEAN_MODEL	Type of ocean model	STRING	MOM4 ▼
OCEAN_RAD	Ocean radiation model	BOOLEAN	MOM4
			MIT-OGCM
BIO_CHEM	Biochemistry	BOOLEAN	Data model
SEA_ICE	Sea ice	STRING	CICE

Goal: Simplify tedious work needed for scientists to perform complex model runs and data management



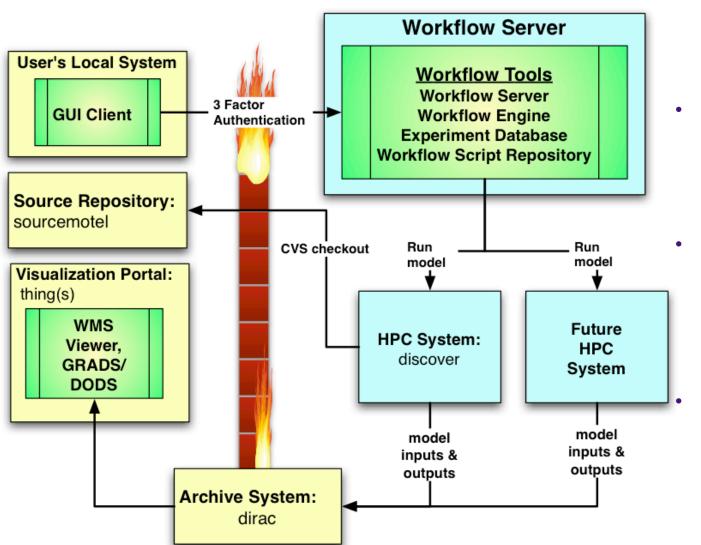


- Remove user from having to manage the system environment
- Clearly present model and runtime options
- Detect common configuration errors early
- Automate the complex tasks underneath
- Provide other tools through an end-to-end chain (configuration to monitor/control to visualization/analysis)
- Make experiments repeatable and shareable

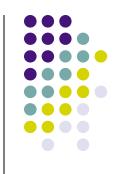


Workflow System at NASA





- Run many types of workflows from a single location
 - Connects to HPC resources under the hood in order to perform tasks
 - Works under high-security environments



NASA Experiment Designer & Light-Weight Workflow Engine

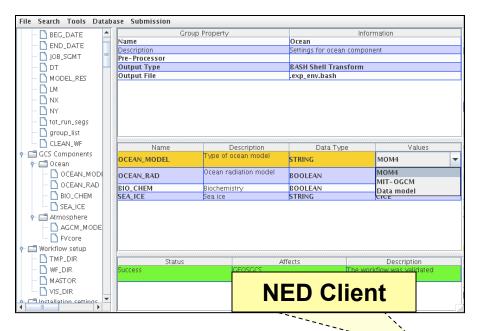
NED & LWWE

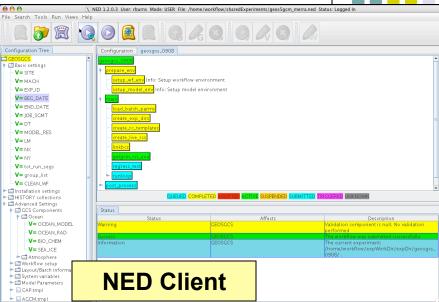


- Client/server
- Componentized, pluggable architecture for adding new features
- Written in Java (portable)
- XML data formats
- Security features
 - Uses encrypted SSL socket communication
 - Performs LDAP and Radius authentication with NCCS servers

Workflow Tool Components







Searchable Experiment

Database or XML File

Configuration Template

Version-Control Repository

Base "Run" Scripts

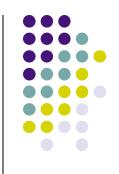
NED Server (Configure/ Control)

Configuration

Status

LWWE (Scheduler)

Workflow



GEOS5 Workflow: Recent Work

GEOS-5 CVS Tags



- Added support for:
 - GEOSagcm-Eros_7_24
 - GEOSagcm-Eros_7_25
 - Other tags can be tested, but not yet fully supported
- Tagged experiments can be checked out, built and run from the Workflow tool
- Obtained restart files for supported tags
- Workflow automatically creates the build and run environments according to tag

GEOS5 Fortuna Workflow



- Now support Fortuna-1_3 tag from the Fortuna module of GEOS5
- User selects the CVS module (either GEOSagcm or Fortuna)
- Fortuna compatible restart files acquired and archived
- New aeroclim, optics and other boundary conditions supported
- Added support for .nc4 file formats

GEOS5 Workflow



- "Pythonization" of GEOS5 workflow scripts
 - Converted from bash scripts currently used in workflow
 - Why? Increased flexibility, reuse, error handling and execution security
 - Updated scripts per code review from the team
 - Tested workflow for the comparison with the original workflow used in bash
- See the next slide for the example

GEOS5 Workflow

Showing python and bash scripts for the comparison

```
# Performs the notification task that has option of emailing.
# Exception will be thrown if any failure of email or missing key.
                                                                                        . $NED WORKING DIR/.exp env.bash
                                                                                        # Check for the email option
def notification(self):
                                                                                        echo -e "\nEMAIL OPTION: $EMAIL OPTION"
    # Check for the email option
                                                                                        if [ "$EMAIL_OPTION" != "true" ]; then
    print "\nEMAIL_OPTION: %s" % self.vars['EMAIL_OPTION']
                                                                                          echo "INFO: no emailing"
    if self.vars['EMAIL_OPTION'] != 'true':
                                                                                          exit 0
      print "INFO: no emailing"
                                                                                        fi
      return
                                                                                        # Create the script file for email
    # Set up the email
                                                                                        echo -e "\nCreating the script file for emailing"
    print "\nStarting to email for notification..."
                                                                                        EMAIL FILE=email.bash
    nedID = self.vars['NED_UNIQUE_ID']
                                                                                        EMAIL_PATH=$NED_WORKING_DIR/$NED_UNIQUE_ID/bin
    email = "%s@nccs.nasa.gov" % self.vars['NED_REAL_USER']
                                                                                        EMAIL_FULL=$EMAIL_PATH/$EMAIL_FILE
    echoCmd = "echo -e \"Subject: %s\\n%s is completed.\"" % (nedID,nedID)
    mailCmd = "/usr/bin/mail" + email
                                                                                        echo "EMAIL FILE: $EMAIL FILE"
    sysCmd = "%s I %s" % (echoCmd, mailCmd)
                                                                                        echo "EMAIL_PATH: $EMAIL_PATH"
    errCode = os.system(sysCmd)
                                                                                        echo "EMAIL FULL: $EMAIL FULL"
    print "\nStatus for %s: %d" % (sysCmd, errCode)
    if errCode:
                                                                                        echo "#!/bin/bash" > $EMAIL_FULL
      raise EnvironException("Failure of notification")
                                                                                        echo "export NED_REAL_USER=$NED_REAL_USER" >> $EMAIL_FULL
    print "\nDone with notification."
                                                                                        echo "export NED UNIQUE ID=$NED UNIQUE ID" >> $EMAIL FULL
                                                                                        echo "export SUBJECT=$NED_UNIQUE_ID" >> $EMAIL_FULL
                                                                                        echo "export EMAIL=$NED_REAL_USER@nccs.nasa.gov" >> $EMAIL_FULL
```

echo "echo \"Workflow \\$NED UNIQUE ID' is complete.\" I /usr/bin/mail -s \"\

\$SUBJECT\"\\$EMAIL">>> \$EMAIL_FULL

echo -e "Done with creating the script file for emailing\n"

chmod +x \$EMAIL FULL

GEOS 5 Workflow



- Current development Lightweight Workflow Engine (LWWE) conversion
 - Created the workflow architecture in XML and tested simple tasks including scripts.
 - Continue with converting the GEOS5
 Workflow used in LWWE from SMS.
 - Why to use LWWE?
 - Flexibility and improved performance